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TECHNICAL REPORT ARBRL-TR-02544

DERIVATION OF THE P^2_T CRITERION (IN CLOSED
FORM) BASED ON THE FREY SHEAR BAND
MECHANISM

Evan Harris Walker

January 1984



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I. INTRODUCTION

In a previous report,¹ an expression for the shear band shear velocity in a shock loaded homogeneous di-constituent explosive was derived and used with the Frey shear band theory of explosive initiation to calculate values of P^2T for explosives, where P is the pressure to which the explosive is shock loaded and T is the temporal duration of the applied pressure. In that treatment, the origin of the P^2T condition as such was not derived. The approach used a computer code developed by R. Frey² (Explosive Effects Branch, Terminal Ballistics Division, Ballistic Research Laboratory) to solve the problem of heat evolution and exchange during the growth of shear bands. In the present paper, approximate expressions are obtained for the development of the shear bands which are used to obtain a closed form expression for the P^2T criterion. Such an expression, though approximate, has great utility in exhibiting the important parameters that determine the sensitivity of an explosive in terms of the physical and thermodynamic properties of that explosive.

The P^2T criterion for the onset of detonation was first proposed by Walker and Wasley.³ The criterion has been extensively studied and supported by experimental data.⁴⁻⁹ The criterion is essentially equivalent to the critical total energy fluence ϵ (since $\epsilon = \rho_0 u^2 t$; u being the particle velocity, and $p = \rho_0 u v$, ρ_0 being the ambient explosive density, we obtain $\epsilon = p^2 t / \rho_0 v$; $\rho_0 v$ is nearly constant for pressures of interest). An understanding of the processes by which initiation of detonation occurs requires an understanding of the P^2T mechanism.

¹E. H. Walker, "Use of the Shear Band Initiation Model to Compute Critical P^2T Values for Explosives," BRL Technical Report (in preparation).

²R. B. Frey, "The Initiation of Explosive Charges by Rapid Shear," *Seventh Symposium (International) on Detonation*, pp 53-59, 16-19 Jun 81, Annapolis, MD.

³F. E. Walker and R. J. Wasley, "Critical Energy for the Shock Initiation of Heterogeneous Explosives," *Explosivestoffe* 17, 9 (1969).

⁴P. Howe, R. Frey, B. Taylor, and V. Boyle, "Shock Initiation and the Critical Energy Concept," *Sixth Symposium (International) on Detonation*, pp 11-19, ACR-221, US Government Printing Office, Washington, D.C., 20402.

⁵E. F. Gittings, "Initiation of a Solid High Explosive by a Short Duration Shock," *Fourth Symposium (International) on Detonation*, pp 373-380, ACR-126, US Government Printing Office, Washington, D.C., 20402.

⁶E. L. Lee and C. M. Tarver, "Phenomenological Model of Shock Initiation in Heterogeneous Explosives," *Phys Fluids* 23, 2362-2372 (1980).

⁷R. C. Weingart, R. K. Jackson, C. A. Honodel, and R. S. Lee, "Shock Initiation of PBX9404 by Electrically Driven Flyer Plates," *Tenth Symposium on Explosives and Pyrotechnics*, preprint UCRL-82162, Jan 79.

⁸Y. de Longueville, C. Fauquignon, and H. Moulard, "Initiation of Several Condensed Explosives by a Given Duration Shock Wave," *Sixth Symposium (International) on Detonation*, pp 105-114, ACR-221, US Government Printing Office, Washington, D.C., 20402.

⁹E. H. Walker, "Computer Model of Shield Design for Artillery Shell Fratricide Suppression," BRL Technical Report (in preparation).

A number of studies¹⁰⁻¹⁴ have sought to derive or calculate values for the P^2T criterion, but none has provided a strictly physical theory free of ad hoc assumptions as to the origin and distribution of initiation sites, "hot spots," or the assumed initiation temperature distribution behind the shock front. The necessity of the "hot spot" concept of Bowden¹⁵ and Eyring¹⁶ comes from the fact that, under shock initiation conditions, the bulk temperature of the explosive produced by adiabatic compression is generally much too low to ignite the explosive. Bowden and Yoffe¹⁵ developed the theory of adiabatic compression of air cavities in the explosive as the source of the hot spots. (See also the work of Starkenberg.¹⁷) Mader¹⁸ has suggested void closure in the explosive as the mechanism for hot spot formation and Seeley¹⁹ has suggested jetting during void closure. Delpuech, et al,²⁰ have proposed shock induced free radical formation as the mechanism underlying hot spot formation. Nevertheless, these mechanisms have not been tied to a P^2T criterion. The shear band mechanism proposed by Frey,² however, has been used to calculate¹ the critical value of P^2T for Composition-B. It is therefore important to tie the shear band mechanism for hot spot formation directly to the condition that the critical value of P^2T for an explosive is a constant.

¹⁰ See References 3, 6, 8.

¹¹ B. O. Trott, R. G. Jung, "Effect of Pulse Duration on the Impact Sensitivity Of Solid Explosives," *Fifth Symposium (International) on Detonation*, pp 191-205, ACR-184, US Government Printing Office, Washington, D.C., 20402.

¹² J. Wackerle, J. O. Johnson, and P. M. Halleck, "Shock Initiation of High-Density PETN," *Sixth Symposium (International) on Detonation*, pp 20-28, ACR-221, US Government Printing Office, Washington, D.C., 20402.

¹³ D. B. Hayes, "A P^2T Detonation criterion from Thermal Explosion Theory," *Sixth Symposium (International) on Detonation*, pp. 76-81, ACR-221, US Government Printing Office, Washington, D.C., 20402.

¹⁴ W. H. Andersen, "Model of Impact Ignition and Explanation of Critical Shock Initiation Energy II Application," *Seventh Symposium (International) on Detonation*, pp 219-225, 16-19 Jun 81, Annapolis, MD.

¹⁵ F. P. Bowden and A. D. Yoffe, *Initiation and Growth of Explosions in Liquids and Solids*, Cambridge University Press (1952).

¹⁶ H. Eyring, R. E. Powell, G. H. Duffrey, and R. B. Darlin, *Chemical Review* 45, 69 (1949).

¹⁷ J. Starkenberg, "Ignition of Solid High Explosive by the Rapid Compression of an Adjacent Gas Layer," *Seventh Symposium (International) on Detonation*, pp 1-12, 16-19 Jun 81, Annapolis, MD.

¹⁸ C. L. Mader, *Phys Fluids* 8, 10 (1965).

¹⁹ L. B. Seeley, "A Proposed Mechanism for Shock Initiation of Low Density Granular Explosives," *Proceedings of the Fourth Electric Initiator Symposium* (1963).

²⁰ A. Delpuech, J. Cherville, and C. Michaud, "Molecular Electronic Structure and Initiation of Secondary Explosives," *Seventh Symposium (International) on Detonation*, pp 36-44, 16-19 Jun 81, Annapolis, MD.

II. WORK DONE BY SHEAR FORCES

The work W per unit volume done in shearing is given by the general expression

$$dW = \sum_i \sum_j \sigma_{ij} d\epsilon_{ij} \quad (1)$$

where σ_{ij} is the shear stress in the plane normal to the x_i - axis directed along the x_j - axis of a Cartesian coordinate system, and ϵ_{ij} is the corresponding strain. If we have shears only on surfaces normal to the y - axis, directed only in the z direction, with the corresponding strains, we can write simply

$$dW = \sigma_{yz} d\epsilon_{yz} \quad (2)$$

The shear stress for a viscoplastic material for such a flow is

$$\sigma_{yz} = \mu \frac{dv_z}{dy} + \sigma_s \quad (3)$$

where v_z is the shear velocity in the direction of the z - axis varying in the y direction. The strength of the material is given by σ_s , while μ is the viscosity. The development of the shear bands takes place in essentially two stages: (1) initial development of shear failure planes and (2) viscous heating of the shear layers. In the first stage, the material undergoes elastic deformation up to shear failure, so that the viscosity term in Equation (3) plays no role; and in the second stage the shear strength drops to zero:

$$\sigma_s = 0 \quad (4)$$

During stage two, the principal heating phase, we can re-express Equation (3) as

$$\sigma_{yz} = \mu dv_z/dy = \mu \frac{\delta(dZ/dt)}{\delta y} = \mu \frac{d\delta z}{\delta y dt} \quad (5)$$

or writing ϵ_{yz} for $\delta z/\delta y$ and rearranging

$$d\epsilon_{yz} = \frac{1}{\mu} \sigma_{yz} dt \quad (6)$$

Therefore, we can substitute for $d\epsilon_{yz}$ in Equation (2) to obtain, on integrating

$$W = \frac{1}{\mu} \int \sigma_{yz}^2 dt \quad (7)$$

III. THE SHEAR VELOCITY IN DI-CONSTITUENT EXPLOSIVES

Walker¹ has given an expression for the shear velocity in an explosive consisting of two materials. For a matrix material having density ρ_1 and sound velocity u_1 containing grains with density ρ_2 and sound velocity u_2 , a shock pressure p gives rise to particle velocities v_1 and v_2 satisfying

$$p = \rho_1 u_1 v_1 = \rho_2 u_2 v_2 \quad (8)$$

Therefore, the shear velocity v_s , the difference between v_1 and v_2 is

$$v_s = p \left(\frac{\rho_2 u_2 - \rho_1 u_1}{\rho_1 u_1 \rho_2 u_2} \right) \quad (9)$$

As shown in Figure 1, the shear velocity initially causes a strain to develop in the matrix material. (A similar process occurs in the grains.) Where $2n$ is the number of shear bands in the spacing of $2D$ between grains in the explosive mixture, at a time t the strain $n\delta d$ (as shown in Figure 1) will be

$$n\delta d = v_s t \quad (10)$$

and also the number of bands between the wall and center between grains is given in terms of the average band spacing d by

$$n = D/d \quad (11)$$

When the strain $\delta d/d$ reaches a critical distortion angle θ_{\max} ,

$$\delta d/d = \theta_{\max} \quad (12)$$

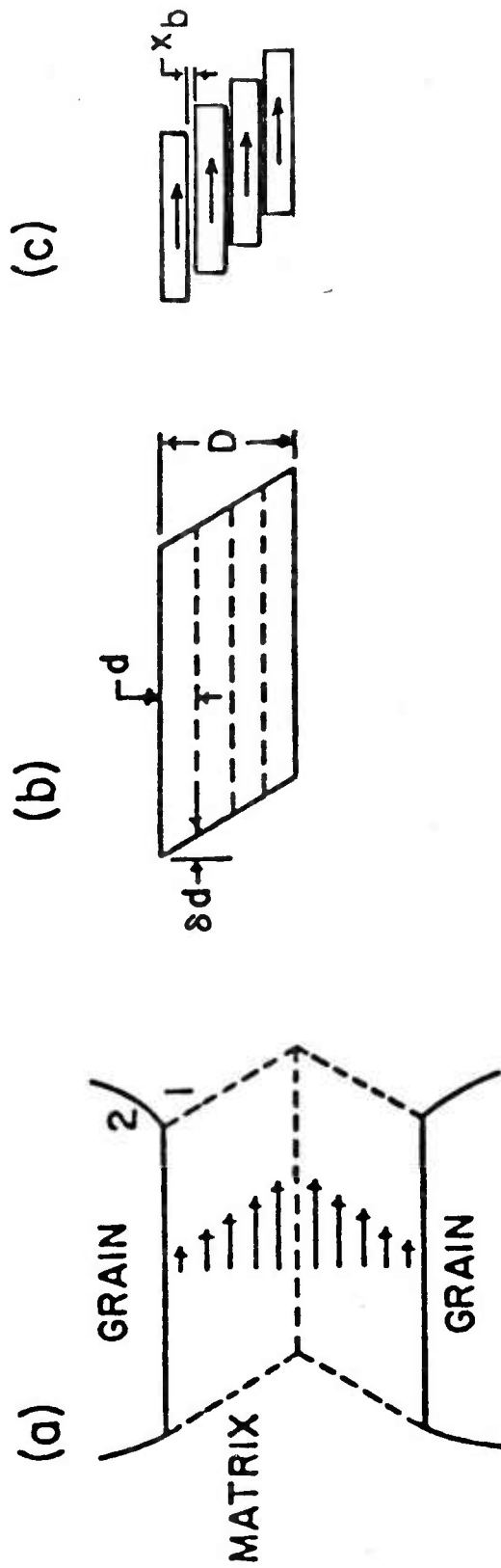


Figure 1 - Schematic diagram showing (a) the differential velocity field produced behind a shock passing through a di-component explosive, (b) a detail of the initial strain due to the differential velocity flow (exaggerated), and (c) a schematic of the shear bands of thickness x_b separated by unsheared material of thickness d .

shears develop in the material. As shears begin to develop, however, stress relief waves propagate from these incipient shears into the surrounding material. This means that the next nearest shear will be located on the average a distance $u_1 t$ away. Since this distance is also d we have

$$u_1 t = d, \quad (13)$$

so that solving we have

$$d = \theta_{\max} D u_1 / v_s \quad (14)$$

θ_{\max} can be re-expressed in terms of Poisson's ratio ν , the ultimate shear strength σ_{\max} and the Young's elastic modulus E by

$$\theta_{\max} = 2(1 + \nu) \sigma_{\max} / E \quad (15)$$

The width of the band when $\sigma_s \rightarrow 0$ can be calculated in terms of the heat made available by the formation of these shears during the time t in which the shear banding structure forms. Thus, using energy conservation to determine the thickness of the layer heated, we write,

$$x_b \rho_1 Q_f = \sigma_{\max} v_b t \quad (16)$$

where Q_f is the latent heat of fusion and v_b , the shear velocity for a single band, is given by

$$v_b = v_s / n \quad (17)$$

Thus, we obtain for x_b

$$x_b = \frac{\sigma_{\max} \theta_{\max} D}{n \rho_1 Q_f} \quad (18)$$

or, substituting from Equation (15),

$$n x_b = 2 (1 + \nu) D \sigma_{\max}^2 / \rho_1 Q_f E \quad (19)$$

From Equations (9) and (19) we can obtain the average velocity gradient across the shear:

$$\frac{dv_z}{dy} \approx \frac{v_z}{nx_b} = p \frac{\rho_1 Q_f E}{2(1+\nu) D \sigma_{\max}^2} \left(\frac{\rho_2 u_2 - \rho_1 u_1}{\rho_1 u_1 \rho_2 u_2} \right) \quad (20)$$

This expression can then be used to obtain σ_{yz} from Equation (3) where Equation (4) holds.

IV. THE P^2T CONDITION

Substituting from Equation (20) into Equation (3) with σ_s set to zero, we have

$$\sigma_{yz} = p \frac{\mu \rho_1 Q_f E}{2(1+\nu) D \sigma_{\max}^2} \left(\frac{\rho_2 u_2 - \rho_1 u_1}{\rho_1 u_1 \rho_2 u_2} \right) \quad (21)$$

Substituting this expression for σ_{yz} into Equation (7) gives

$$W = \mu \left[\frac{\rho_1 Q_f E}{2(1+\nu) D \sigma_{\max}^2} \left(\frac{\rho_2 u_2 - \rho_1 u_1}{\rho_1 u_1 \rho_2 u_2} \right) \right]^2 \int p^2 dt \quad (22)$$

where the constants (or slowly varying parameters) have been factored from under the integral.

The energy W (per unit volume) goes into heating the material in the shear band. Where ΔT_{ig} is the temperature rise above the melt temperature required to bring the matrix to the "ignition temperature," we can express the critical value for W by

$$W_{\text{crit}} = \rho_1 C_v \Delta T_{ig} \quad (23)$$

where C_v is the specific heat of the matrix material. Strictly speaking, there is no specific ignition temperature. Instead, there exists a relationship, the Arrhenius equation, relating rate of heat evolution to the temperature of the explosive. However, for the shock loading times of major interest, i.e., in the range of 1-100 μs , the dependence of T_{ig} on the shock loading time varies slowly. Heat evolution rises exponentially with temperature, which in turn further elevates the explosive temperature; as a result, the initial temperature necessary to produce complete combustion within the shear band in a time of 1 μs will differ very little from that required for complete combustion in 100 μs . For this reason we can ignore the dependence of T_{ig} on shock loading time in order to retain a closed form expression for W_{crit} . Defining

Q_h as the P^2 time integral for the shear band heating phase, we have from Equations (22) and (23):

$$Q_h \equiv \int p^2 dt = \frac{C_v \Delta T_{ig}}{\rho_1 \mu} \left[\frac{2(1+\nu) D \sigma_{max}^2}{Q_f E} \left(\frac{\rho_1 u_1 \rho_2 u_2}{\rho_2 u_2 - \rho_1 u_1} \right) \right]^2 \quad (24)$$

Equation (24) provides an approximate expression for the P^2T criterion in terms of the physical and thermodynamic properties of an explosive under the conditions of matrix initiation. A corresponding expression for grain initiation may be given in which D and σ_{max} are calculated for grain shearing. The P^2T criterion is given by the expression in Equation (24) if the matrix goes into shear before the grains, as in Composition-B. If the grains shear with the matrix deforming, the quantities ρ_2, u_2 will be for the matrix and all other quantities for the grains.

Matrix (TNT)	C_v	=	$1.29 \times 10^5 \text{ J/Kg}^{\circ}\text{K}$
	ΔT_{ig}	=	$T_{ig} - T_{melt} = 720^{\circ}\text{C}$
	ρ_1	=	$1.63 \times 10^3 \text{ Kg/m}^3$
	u_1	=	$2.08 \times 10^3 \text{ m/s}$
	μ	=	$1.39 \times 10^{-2} \text{ Kg/ms}$
	ν	=	0.3

For Composition-B we have the values:

D	=	$5 \times 10^{-6} \text{ m}^{(21)}$
σ_{max}	=	$7.0 \times 10^7 \text{ Pa}$
Q_f	=	$8.96 \times 10^4 \text{ JKg}$
E	=	$5.4 \times 10^9 \text{ Pa}$

Grain (RDX)	ρ_2	=	$1.8 \times 10^3 \text{ Kg/m}^3$
	u_2	=	$2.65 \times 10^3 \text{ m/s}$

These values yield

$$Q_h = 9.8 \times 10^{12} \text{ Pa}^2 \text{ s} \quad (25)$$

In addition to the frictional heating in the shear bands, once ignition of the explosive at these hot spots has occurred, combustion must continue if a detonative shock pressure is to form. If a rarefaction wave arrives too early, in the process, the rate of heat evolution will drop and cooling or mechanical dispersal of the explosive can extinguish the ignition process. Therefore, if the burn is to be maintained, the externally applied shock pressure must be maintained until this external source of pressure is replaced by internal sources. The internal sources, of course, must be the hot spots which generate pressure by combustion. We require that the externally applied pressure p be maintained for a time t_b sufficiently long that,

²¹See Appendix A.

if at the end of this time the external pressure is relieved, the internal pressure will just match that loss of pressure. (Note that this internal pressure will not lead to mechanical disruption of the explosive until a relief wave can arrive from the explosive surface.) Since we are concerned with compact explosives here, the energy density is equal to the pressure generated. Thus, to produce a pressure p from the combustion of an explosive having a "bomb" pressure (bomb at full density) p^* , a fraction p/p^* must be burned. Where U_b is the burn velocity and d the distance between shear bands, we require

$$p/p^* = U_b t_b / (1/2 d) \quad (26)$$

Thus, the total P^2T value of the critical condition for explosive initiation will be

$$Q_{tot} = Q_h + Q_b \quad (27)$$

where Q_b is given by

$$Q_b = p^2 t_b = p^3 d / 2U_b p^* \quad (28)$$

Of course, the burn velocity U_b is itself a function of the pressure. Kondrikov, Raikova, and Samsonof²² give

$$U_b = \rho B p^v \quad (29)$$

where ρ is the explosive density, p the pressure, B and v are constants with values $B=0.0219\text{g/cm}^2\text{s atm}^v$ (20-100 Atm), $= 0.0094\text{g/cm}^2\text{s atm}^v$ (100-450 Atm); $v = 0.77$ (20-100 Atm), $= 0.95$ (100-450 Atm). We obtain p^* for TNT using the TIGER computer code²³ giving $p^* = 9.67 \times 10^9$ Pa. At 10 kbar, (2.03×10^8 Pa), $U_b = 0.21$ m/s so that $Q_b = 2.79 \times 10^{11}$ Pa²s. Since U_b is approximately proportional to pressure, Q_b varies quadratically with the pressure. Thus, Q_b will not be as important as Q_h until we reach shock pressures of more than 6.75×10^9 Pa (67 kbar). This latter value is only approximate since this pressure lies outside the range for which values of U_b are accurate. The critical P^2T value obtained experimentally is 4.41×10^{12} Pa²s. Thus, the theoretical value, Q_{tot} , for the P^2T criterion as given in Equation (25) is reasonably good.

²² B. N. Kondrikov, V. M. Raikova, and B. S. Samsonof, Fizika Goreniya i Vzryva, 9 #1, 84-90 (1973).

²³ M. Cowperthwaite and W. H. Zwisler, TIGER Computer Program, SRI International Publication No. Z106, SRI International, 333 Ravenswood Ave, Menlo Pk, CA 94025.

V. CONCLUSIONS

We have obtained an approximate closed form expression for the P^2T criterion for explosive initiation based on the shear band theory of explosive ignition. While the resulting expression depends on quantities that are only poorly known in many cases, the equation exhibits explicitly the factors controlling explosive sensitivity. The resulting equation shows a dependence of the P^2T criterion on particle size for fixed mass fractions of the constituents, and for fixed particle size, shows P^2T increases as the portion of matrix (TNT in Comp B) is increased. The P^2T criterion equation obtained here exhibits explicitly the important parameters determining the sensitivity of an explosive in terms of its physical and thermodynamic properties.

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21. See Appendix A.
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APPENDIX A

CALCULATION OF AVERAGE GRAIN SIZE OF RDX IN COMPOSITION-B

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CALCULATION OF AVERAGE GRAIN SIZE OF RDX IN COMPOSITION-B

The value of D, the average grain diameter used in Equation (25) was obtained from data for the composition-B shown in Figure 2 of Reference 1. The data are given in Table A1.

TABLE A1

Percent of RDX having Grain Sizes in the Indicated Size Ranges

<u>Percent RDX (%)</u>	<u>Size Range (μm)</u>
2.0	> 900
9.8	> 350
35.3	> 200
39.7	> 100
13.2	< 100

To use these data to obtain D, we must make an assumption as to the packing of the grains and their shape. We assume the grains to be spherical and equally spaced in a close packed hexagonal arrangement. This does not mean that the grains are in contact but that each grain of radius r_g at the center of a sphere of radius R, which we can treat as pseudograins in contact with each other in the close packed hexagonal arrangement. The volume of a grain is

$$V_{\text{grain}} = \frac{4}{3} \pi r_g^3 \quad (\text{A1})$$

The volume of a pseudograin is

$$V_{\text{pseudo}} = \frac{4}{3} \pi R^3 \quad (\text{A2})$$

and the quantities R, r_g , and D are related by

$$D = R - r_g \quad (\text{A3})$$

The volume of a cell containing one pseudograin for the close packed hexagonal arrangement (boundaries of the cell are defined by the tangent planes at the points of contact between spheres) is

$$V_{\text{cell}} = 4\sqrt{2} R^3 \quad (\text{A4})$$

Therefore, g is given by

$$g = V_{\text{grain}}/V_{\text{cell}} = \pi r_g^3 / 3 \sqrt{2} R^3 \quad (\text{A5})$$

For the mass fraction, we note that the masses of the grain, M_{grain} , and matrix, M_{matrix} , are given in terms of the respective densities, ρ_{grain} and ρ_{matrix} , by

$$M_{\text{grain}} = \frac{4}{3} \pi \rho_g r_g^3 \quad (\text{A6})$$

and

$$M_{\text{matrix}} = \rho_{\text{matrix}} \left[4 \sqrt{2} R^3 - \frac{4}{3} \pi r_g^3 \right] \quad (\text{A7})$$

With the mass fraction of the grain material being g_m , we have

$$g_m = \frac{\pi \rho_g r_g^3}{3 \sqrt{2} \rho_{\text{matrix}} R^3 + \pi (\rho_{\text{grain}} - \rho_{\text{matrix}}) r_g^3} \quad (\text{A8})$$

From the data in Table A1 we can obtain the weighted value of $\overline{r_{\text{grain}}^2}$:

$$\overline{r_g^2} = \frac{\sum w_i \frac{1}{r_g^3} r_g^2}{\sum w_i \frac{1}{r_g^3}} = (5.65 \times 10^{-5} \text{ m})^2 \quad (\text{A9})$$

where the term $1/r_g^3$ represents the grain weights, w_i their percentages and r_g^2 is used since we seek the value of D^2 for use in Equation (24). Where $g_m = 0.6$, $\rho_{\text{grain}} = 1.80 \text{ g/cm}^3$, and $\rho_{\text{matrix}} = 1.63 \text{ g/cm}^3$, Equations (A8) and (A3) can be solved to obtain

$$D = 4.94 \times 10^{-6} \text{ m} \quad (\text{A10})$$

which was rounded off to $5 \times 10^{-6} \text{ m}$ for use in Equation (24).

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